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**New Exchange-Correlation Potentials for Quantum
Transport and Other Non Equilibrium Processes as
Described by Time-Dependent Density Functional Theory**

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| 14. ABSTRACT <p>With the work performed in this research project, some fundamental aspects of TDDFT for strongly correlated systems have been characterized from several perspectives, such as the role of the exchange-correlation discontinuity in metal-insulator transitions and in quantum transport, the limitations but also the merits of adiabatic approximations, the necessity to include memory and nonlocal effects, to mention a few. Furthermore, the pioneering direction of research initiated within this project, namely TDDFT for strongly correlated lattice models, has in fact turned into an active subfield of TDDFT, with several papers and different authors contributing to the field, with new theoretical schemes, new theorems specifically proven for lattice (TD)DFT, applications to "distant" areas such as ultracold atoms, Kondo physics (for a recent review, see paper 12, App. B). It is fair to say, that our and other's work has so far barely grasped the surface. Several possible directions can be easily envisaged to continue research in TDDFT: introducing memory and non local effects in the XC potentials (possibly exploiting more closely the connection with Kadanoff-Baym dynamics), magnetism in strongly correlated systems, electron-phonon interactions, etc. In particular, one important aspect, mentioned in the grant proposal and not significantly developed in the period covered by the grant, is the actual implementation of TDDFT within the ab-initio SeqQuest code. This aspect was only partially dealt with during the grant period (a large amount of preliminary work was done in this respect, but no concrete implementation is available and/or in close sight), and remains a priority in the future research plans of the principal investigator. To summarize, the research carried out during the grant period has provided a solid and attractive education profile to the PhD student Alexey Kartsev. It has also showed the great potential of TDDFT in describing the non-equilibrium dynamics of strongly correlated materials, and that there are many stimulating problems to be addressed in order to further develop an important approach such as TDDFT.</p> | | | | | | |
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Final report on the Scientific Activity for the Research Grant FA8655-08-1-3019. Principal Investigator: Claudio Verdozzi

Overview

The central aim of the project was to devise new exchange-correlation functionals for a time-dependent density-functional theory (TDDFT) approach to condensed-matter systems in out-of-equilibrium with strong correlation effects among the electrons, and possibly to consider also interactions between electrons and lattice vibrations. An important aspect of the project was to hire of a PhD student to perform research of relevance to the project. According to the regulations of the host institution (Lund University), the funding from the grant covered three of the four years of the PhD student activities, the remaining one year (and slightly more) being funded by the host institution (Lund University). The present final report provides i) a complete summary of the student's activities in the entire period of the grant; ii) a complete summary of the activities of the principal investigator (CV) in the same period; iii) lists of publications and participations to conferences and related activities, of relevance to the topics of the grant; iv) final considerations about the outcomes of the project and an outlook.¹

1. The PhD student's activity

Alexey Kartsev, the PhD student devoted to the project, was hired in March 2008, after a selection process through more than seventy applicants. However, having to finish his activities in Moscow, the start of his PhD in Lund was postponed to mid October 2008. Alexey Kartsev is expected to obtain his PhD in Spring 2013.

1.a Education

During his PhD thesis, and in compliance with Lund University regulations, Alexey has attended several PhD courses, and passed with proficiency the inherent exams. These courses, which were intended to enhance his scientific education, and integrate the large number of advanced courses already taken by Alexey during his undergraduate studies in Moscow, were: Advanced Solid State Theory, Electromagnetism, Quantum Information, Many-Body Theory, Superconductivity and Superfluidity, Quantum transport, Parallel computing, and Quantum Mechanics for Modern Devices. Furthermore, he has had substantial private lecturing from CV on several subjects of relevance to the project, such as time-dependent quantum mechanics, static and time-dependent density-functional theory, electronic structure calculations, physics of strongly correlated systems and ultracold atoms in optical lattices, recursion techniques, numerical solution of model Hamiltonians, exact static and time-dependent methods, group theory, etc.

1.b Research

A main goal of this project was to devise new exchange-correlation functionals for strongly

¹ For sake of completeness, in the present, comprehensive and final account, parts from previous interim reports were included, and some overlap can be noted at a number of places. Since the last interim report, the new activity consisted in the work inherent the papers 12, 13 listed in Appendix B, as discussed in the main text.

correlated systems. These studies are of considerable pedagogical value, since they provide profound and novel insight into how to proceed for an ab-initio formulation. Within the project, Alexey has developed spin-dependent exchange-correlation (XC) potentials for 1D strongly correlated systems. He has then applied these potentials to study the competition of disorder and interaction effects in quantum transport, to spin transport, and to ultracold atom physics in 1D. He has further developed and used XC potentials for 3D lattice systems to the study of expansion of trapped fermionic clouds in 3D in the presence of disorder. Such activities are detailed below. In the Fall 2012 the results of his work will be presented at two conferences.

1.b.1 Development of exchange correlation potentials.

In the projects considered here, one needs XC potentials that are 1) spin-dependent, and 2) they account properly for strong electron-electron correlations. An important part of Alexey's initial activity has been producing and testing spin-dependent XC potentials. These were obtained via the use of Bethe-Ansatz theory, which permits an exact treatment of the 1D homogeneous Hubbard model, which is a strongly interacting system. The Bethe-Ansatz solution was obtained by solving numerically two coupled integral equations (for the spin and the charge densities, respectively). For this, Alexey developed a completely new computer code, which required the use of several numerical techniques for differentiation, integration and interpolation. Alexey has tested the XC potentials thus obtained against exact calculations, with very encouraging results. Alexey has also started to use these potentials in specific applications, as discussed next.

1.b.2 Exploring localization and transport properties with (TD)DFT.

The XC potentials developed by Alexey were then used to investigate the static and dynamical behavior of interacting fermions in short disordered chains contacted to semi-infinite leads. The main aim of this study was to characterize the joint role of disorder and interactions. A definition of the inverse participation suitable for quantum transport geometries was used as indicator of localization within (TD)DFT. Merits and limits of the coherent-potential approximation were also studied. The results, submitted to the journal *Physical Review B* (paper 12 in Appendix A), showed a dynamical enhancement of delocalization in presence of a finite bias, and an increase of the steady-state current induced by inter-particle interactions. While similar behavior is well known in the ground state, in this work it was observed for the first time in the non-equilibrium regime, and within TDDFT.

1.b.3 Spin transport in spin-impurity+leads geometries.

This project focuses on spin-dependent transport, such as the effect of ferromagnetic leads, non collinearity, spin-dependent biases and gate voltages, time-dependent spin-blockade. For this project, Alexey performed a considerable amount of code development, to generalize an existing quantum transport code to include electron-electron interactions and spin-dependent perturbations. This required the implementation of a predictor-corrector scheme for the time evolution, within an embedding scheme for spin-dependent leads, for collinear and non-collinear spin geometries. At the moment of writing, preliminary calculations have been performed for double spin impurity systems. The activities of this research will be reported in a manuscript, which will represent the first ever application of TDDFT to time-dependent spin transport in systems with strong correlations.

1.b.4 Ultracold atom physics.

In the last fifteen years, lattice Hamiltonians have received considerable attention in the context

of the physics of ultracold atoms in optical lattices. By experimentally tuning the lattice parameters, paradigmatic models of condensed matter physics, such as e.g. the Hubbard Hamiltonian, can be experimentally realized, thus providing an ideal playground to study fundamental notions such as quantum phase transitions, interaction quenches, approach to equilibrium.

In his work, Alexey has considered how spin separation could be achieved and/or cancelled, by using fermionic particles trapped in parabolic potentials and described by the Hubbard Hamiltonian. His goal was to study different protocols to remove/develop spin polarization. Results indicated that in these processes there is a strong dependence on system dimensionality. Quite interestingly, Alexey found that complete (de)polarization cannot be achieved in 1D, due to the energy barrier introduced by the exchange-correlation potential.

Another project concerns the competition of substitutional disorder versus interactions in the expansion of initially trapped 3D fermionic clouds in cubic lattices. Recently, it has become possible to simulate with great accuracy disordered lattices, to have an ideal setup to investigate the Anderson transition with/out correlation effects. Alexey used a TDDFT based on dynamical mean-field theory, and considered interactions above and below the Mott threshold and also the presence of disorder. Since the project is computationally expensive (supercells with more than 100,000 sites were considered), additional extensions of the computational toolbox were provided by Alexey, to deal with disorder averaging and also to speed-up the convergence of ground state initial calculations by use of group theoretical methods. The system actually considered was one of the main paradigms of strongly-correlated Fermi systems, i.e. the Mott phase of the Hubbard model. The results showed that at strong coupling, multiple timescales manifest in the dynamic melting of the system, as the Mott plateau persist orders of magnitude longer than the band insulating core. Furthermore, disorder increases the localization but destabilizes the Mott plateau, thus creating an interesting crossover in time. While writing this report, a manuscript is being prepared, to be submitted to the journal *Nature Physics* [paper 13, App. B].

2. Other relevant activities of the principal investigator during the period 2008-2012.

The main goal of this project was to devise new exchange-correlation functionals for strongly correlated systems. The study of time-dependent phenomena via TDDFT for strongly correlated systems is still at an early stage: model systems can be of aid, giving guidelines for ab-initio approaches. An assessment of TDDFT for strongly correlated model systems under strong time-dependent fields is thus highly desirable. Next we report of additional work (i.e. besides the papers 12-13 in App. B from the PhD student, A. Kartsev), which are relevant to the project.

2.a Research in TDDFT

2.a.1 Introducing TDDFT for strongly correlated lattice models.

In the late 2008, CV published a paper discussing the potential of TDDFT for strongly correlated lattice systems out of equilibrium. Using the exact many-body time evolution, CV determined the exact XC potential for small Hubbard model chains exposed to time-dependent fields. In the

same paper, an adiabatic local density approximation for the 1D Hubbard model was also introduced and benchmarked against exact results, to gain insight about approximate XC potentials. This was the first work in the literature where TDDFT is used to perform the non-equilibrium dynamics of lattice models with strong electron correlations (since then, the paper has received about 40 citations, according to NASA-ADS) [paper 1, App. B].

2.a.2 Dynamics of 1D ultracold fermion atoms via TDDFT.

The time evolution of the out-of-equilibrium Mott insulator was investigated numerically through calculations of space-time resolved density and entropy profiles resulting from the release of a gas of ultracold fermionic atoms from an optical trap [paper 7, App. B].

2.a.3 TDDFT vs. Dynamical Mean Field Theory.

In this work, we introduced a new class of exchange-correlation potentials for a static and time-dependent Density Functional Theory of strongly correlated systems in 3D. The potentials were obtained via Dynamical Mean Field Theory; for strong enough interactions, they exhibit a discontinuity at half filling density, a signature of the Mott-Hubbard metal-insulator transition. To our best knowledge, this is at present the only available XC potential that, even if at the model level, is able to reproduce the Mott-Hubbard transition. For time-dependent perturbations, the dynamics was described in the adiabatic local density approximation. Results from the proposed scheme compare very favorably to exact ones in clusters. As an application, we studied Bloch oscillations in the 3D Hubbard model [paper 8, App. B].

2.a.4 Studies of Hubbard Clusters by Means of Static DFT and TDDFT.

In this work, DFT methods were applied to a small Hubbard cluster, where exact calculations can be performed, and a "reverse engineering" technique permits to obtain the exact exchange-correlation potential. We found quite unexpected results during our study, namely that for a chosen set of parameters in our system, a singlet-triplet degenerate ground state occurs, where the density is not representable by non-interacting Kohn-Sham electrons in the ensemble sense. Furthermore, via a time evolution in the adiabatic limit, and starting from a v_0 -representable singlet state (i.e. expressible in terms of a Kohn-Sham image), we also showed how TDDFT approaches such a problematic parameter region, thus providing novel insight into the rather complex, non-local nature of the exchange-correlation functional [paper 11, App. B].

2.a.5 TDDFT and dynamical Coulomb Blockade.

The Coulomb Blockade phenomenon is one of the true hallmarks of electron-electron interactions in mesoscopic and nanoscale physics. In molecular transport, the Coulomb Blockade is due to an electrostatic barrier induced by the electrons in the device, which prevents further electrons from tunneling in. Using TDDFT, the discontinuity of the XC potential in the context of electron transport was investigated and showed intimately related to Coulomb blockade. The related paper was selected for a featured "Viewpoint in Physics", a highly selective online publication of the American Physical Society [paper 5, App. B].

2.b Research in Non-equilibrium Green's functions

We studied the effect of a time-dependent external field on small, strongly correlated clusters, described again by a Hubbard Hamiltonian, by propagating the Kadanoff-Baym equations within

the following approximations: Hartree-Fock, second Born, GW and T-matrix. A comparison was made between the results from these schemes and an exact solution. We found that the T-matrix is far superior to the GW approximation and slightly better than the second Born approximation. In the long time limit, the solutions exhibited an unphysical steady state, which was attributed to the implicit inclusion of infinite order diagrams in a few-body system. [papers 2-3, App. B]

As follow-up, we performed similar investigations in quantum transport geometries (lead-device-lead setups), also addressing the nature and emergence of multiple steady- and quasi-steady-states [paper 4, App. B]. We also used the KBE to describe the propagation of entanglement entropy through an out-of-equilibrium model interacting device in a quantum transport set-up. A remarkable result of our calculations is that the double occupancy, necessary for computing the entanglement, can become negative. This is a shortcoming of approximate, and yet conserving, many-body self-energies. We were able to prove analytically that, among the tested perturbation schemes, the T-matrix approximation is exempt from this problem. Finally, we showed that the entanglement transmission across the device could be tuned by a current flowing through the system [papers 6, 10 in App.B].

2.c Comparative studies of TDDFT and Non-equilibrium Green's functions.

In 2010, CV was invited to write a review article for the special issue “*Open problems and new solutions in time dependent density functional theory*” of the journal “Chemical Physics”. Two aspects of TDDFT, the linear response approach and the adiabatic local density approximation, were examined from the perspective of lattice models. Results were presented for the density response function of the 3D homogeneous Hubbard model, a drawback of the linear response scheme was pointed out and a prescription suggested on how to amend it. Exact, adiabatic-TDDFT and Kadanoff-Baym-Equations densities were mutually compared. The results showed that non-perturbative (in the interaction) adiabatic potentials can perform quite well for slow perturbations but that, for faster external fields, memory effects, as already present in simple many-body approximations, are clearly required [paper 9, App. B].

3. Concluding remarks and Outlook

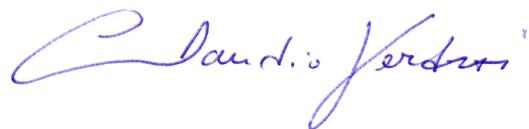
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proposal and not significantly developed in the period covered by the grant, is the actual implementation of TDDFT within the *ab-initio* SeqQuest code. This aspect was only partially dealt with during the grant period (a large amount of preliminary work was done in this respect, but no concrete implementation is available and/or in close sight), and remains a priority in the future research plans of the principal investigator.

To summarize, the research carried out during the grant period has provided a solid and attractive education profile to the PhD student Alexey Kartsev. It has also showed the great potential of TDDFT in describing the non-equilibrium dynamics of strongly correlated materials, and that there are many stimulating problems to be addressed in order to further develop an important approach such as TDDFT.

As conclusive remark, the principal investigator Claudio Verdozzi, also on the behalf of Alexey Kartsev, wishes to express his deepest gratitude to EOARD for providing the support to carry out research for three years in the exciting field of time-dependent density-functional theory.

Lund, August 2012



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APPENDIX A: Conferences, talks and related activities.

These scientific activities pertinent to the aims of the project have met considerable interest within the international scientific community. Since 2008 the main investigator (CV) has participated to several conferences with invited or contributed talks, acted as external PhD examiner and/or reviewer of grant proposals on the topics inherent to the project.

Invited talks

- i) 3rd Workshop on TDDFT (Benasque, 2008).
- ii) Nordforsk Meeting (Kalmar, 2008).
- iii) IFSC workshop on TDDFT (Sao Paulo, 2008).
- iv) International Symposium and Workshop on Correlated Electrons (Gatlinburg, 2009).
- v) Nordforsk Meeting (Copenhagen, 2009).
- vi) Frontiers in Density Functional Theory (Montauk-Long Island, 2009).
- vii) Strongly Correlated Materials (NCES10, Gothenburg, 2010).
- viii) Non-equilibrium phenomena in ultracold atoms (Natal, 2010).
- ix) Theoretical modeling of quantum transport at the nano-scale" (Copenhagen, 2011).
- x) Frontiers of Quantum Mesoscopic Thermodynamics" (Prague, 2011).
- xi) International Symposium and Workshop on Electron Correlations and Materials Properties of Compounds and Alloys (Porto Heli, 2012).
- xii) Progress in non-equilibrium Green's Functions V (Jyväskylä, 2012).
- xiii) CECAM workshop Latest advancements in Green's function theory (Toulouse, 2013).
- xiv) Advances in time-dependent methods for quantum many-body systems (Trento, 2013).

Other conferences and talks

- i) CECAM conference on quantum transport (Lausanne, 2009).
- ii) Gordon Conference on TDDFT (New-Hampshire, 2009).
- iii) KITP conference "From Basic Concepts to Real Materials" (Santa Barbara, 2009).
- iv) Psi-k conference on materials (Berlin, 2010).
- v) Symposium on Cold Atoms and Condensed Matter" (Vedbaek , 2010).
- vi) 16th ETSF Workshop (Turin, 2011).
- vii) Several seminars were given at different institutions.

Other related activities

CV was

- funded within an EOARD Window of Science initiative, to perform a visit to A. H. Edwards (AFR Laboratory-Albuquerque) and P. A. Schultz (Sandia National Labs-Albuquerque) and to give a talk (2009).
- invited to write a review /research article in the special issue of the journal "Chemical Physics.", entitled "Open problems and new solutions in TDDFT" (2010).
- invited to contribute a chapter to a volume "Modern first-principle computational approaches to spectroscopic properties of complex materials." for the series Topics in Current Chemistry edited by Springer (2012).
- invited to be external PhD examiner (thesis opponent) at the University of York (2009), Trinity-College Dublin (2011) and at the University of Jyvaskyla (2012).
- one of the organizers of the workshop "TDDFT in Sweden" (Lund, 2008).
- reviewer for the DFG-German Research Foundation (2008, 2012), the Leverhulme Trust-

London (2010), the Netherlands organization for scientific research (2012), for proposal dealing with TDDFT-based research.

APPENDIX B: Publications relevant to the project for the period 2008-2012

- [1] C. Verdozzi, *Time Dependent Density Functional Theory and Strongly Correlated Systems: Insight From Numerical Studies*, Phys. Rev. Lett. 101, 166401 (2008).
- [2] M. Puig von Friesen, C. Verdozzi, C.-O. Almbladh, *Successes and failures of Kadanoff-Baym dynamics in Hubbard nanoclusters*, Phys. Rev. Lett. 103, 176404 (2009).
- [3] M. Puig von Friesen, C. Verdozzi, C.-O. Almbladh, *Artificial damping in the Kadanoff-Baym dynamics of small Hubbard chains*, J. Phys: Conf. Ser. 220, 012016 (2010).
- [4] M. Puig von Friesen, C. Verdozzi, C.-O. Almbladh, *Kadanoff-Baym description of Hubbard clusters out of equilibrium: performance of many-body schemes, correlation-induced damping and multiple quasi-steady states*, Phys. Rev. B 82, 155108 (2010).
- [5] S. Kurth, G. Stefanucci, E. Koshravi, C. Verdozzi and E. K. U. Gross, *Dynamical Coulomb Blockade and the Derivative Discontinuity of Time-Dependent Density Functional Theory*, Editor's choice, Phys. Rev. Lett. 104, 236801 (2010).
- [6] M. Puig von Friesen, C. Verdozzi, C. -O. Almbladh, arXiv:1009.2917.
- [7] D. Karlsson, C. Verdozzi, M. Odashima and K. Capelle, *Dynamical melting of the Mott insulator: Time evolution of the density and entropy of out-of-equilibrium cold fermion gases*, EPL 93, 23003 (2011).
- [8] D. Karlsson, A. Privitera and C. Verdozzi, *Time Dependent Density Functional Theory meets Dynamical Mean Field Theory: Real-Time Dynamics for the 3D Hubbard Model*, Phys. Rev. Lett. 106, 116401 (2011).
- [9] C. Verdozzi, D. Karlsson, M. Puig von Friesen, C.-O. Almbladh, U. von Barth, *Some open questions in TDDFT: Clues from lattice models and Kadanoff-Baym dynamics*, Chemical Physics, 391, 37 (2011).
- [10] M. Puig von Friesen, C. Verdozzi, C.-O. Almbladh, *Can we always get the entanglement entropy from the Kadanoff-Baym equations? The case of the T-matrix approximation*, EPL 95, 27005 (2011).
- [11] T. Rössler, C. Verdozzi, C. -O. Almbladh, *Studies of Hubbard Clusters by Means of Static and Time-Dependent Density Functional Theory*, in preparation.

[12] V. Vettchinkina, A. Kartsev, D. Karlsson, C. Verdozzi, *Interacting fermions in 1D disordered lattices: Exploring localization and transport properties with lattice density-functional theories*, arXiv:1204.0672 (2012).

[13] A. Kartsev, D. Karlsson, A. Privitera, C. Verdozzi, *Persistence of Mott plateaus in a 3D expansion of a confined Fermi gas into clean and disordered optical lattices*, to be submitted.